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THE KRAMERS-HEISENBERG FORMULA AND THE GUNN-PETERSON TROUGH FROM THE FIRST OBJECTS IN THE UNIVERSE

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ABSTRACT

Recent cosmological observations indicate that the reionized universe may have started at around $z = 6$, where a significant suppression around Lyα has been observed from the neutral intergalactic medium. The associated neutral hydrogen column density is expected to exceed 10^{21} cm^{-2}, where it is very important to use the accurate scattering cross section known as the Kramers-Heisenberg formula that is obtained from the fully quantum mechanical time-dependent second order perturbation theory. We present the Kramers-Heisenberg formula and compare it with the formula introduced in a heuristic way by Peebles (1993) treating the hydrogen atom as a two-level atom, from which we find a devitaion by a factor of two in the red wing region far from the line center. Adopting simple cosmological models, we compute the Gunn-Peterson optical depths and the trough profiles. Our results are compared with the works performed by Madau & Rees (2000), who adopted the cross section introduced by Peebles (1993). We find deviations up to 5 per cent in the Gunn-Peterson transmission coefficient for an accelerated expanding universe in the red off-resonance wing part with the rest wavelength $\Delta\lambda \sim 10$ Å.

Subject headings: cosmology: theory — intergalactic medium – quasars: absorption lines — radiative transfer — galaxies: high-redshift

1. INTRODUCTION

The quasar absorption systems have been excellent tools to investigate the intergalactic medium (IGM), from which it has been well known that the IGM of the nearby universe is highly ionized (e.g. Peebles 1993). Since the universe after the recombination era $z \sim 1100$ should be dominantly neutral, there must be some epoch when the universe began to be re-ionized. Intensive studies have been performed on the emergence of the first objects that ended the dark age of the universe. Numerical calculations adopting the cold dark matter models predicted the reionization epoch in $z \sim 6 - 12$ (e.g. Gnedin & Ostriker 1997).

Around this epoch a broad absorption trough in the blue part of Lyα is expected and regarded as a strong indicator of the reionization of the universe, which was predicted by Gunn & Peterson (1965) and independently also by Scheuer (1965). With the advent of the Hubble Space Telescope and 8 meter class telescopes there have been extensive searches for the Gunn-Peterson trough in the spectra of high red shift objects. Remarkable contributions are made by the Sloan Digital Sky Survey, from which a number of high red shift quasars with z ranging from 4 to 6 have been found. According to the recent report from the Keck spectroscopy of these high red shift quasars (Becker et al. 2001), the flux level drop around Lyα is much higher for the quasar with $z = 6.28$ than those for other quasars with $z < 6$, which indicates that the reionization epoch may be found at around $z \sim 6$.

The exact computation of the flux drop around Lyα requires an accurate atomic physical estimation of the scattering cross section. Recent theoretical works on the calculation of the Gunn-Peterson trough were provided by Miralda-Escudé (1998) and Madau & Rees (2000), who adopted the formula that was introduced in a heuristic way using the second order time-dependent perturbation theory by Peebles (1993). The formula is derived based on the assumption that the hydrogen atom is a two-level atom, in order to show the behavior of the scattering cross section that is approximated by the Lorentzian near resonance and yields ω^4 dependence in the low energy limit. As Peebles noted clearly in the text, due to the two-level assumption, the formula provides an inaccurate proportionality constant in the low energy limit, even though it correctly gives the ω^4 dependence.

The accurate cross section should be obtained from the second order time-dependent perturbation theory treating the hydrogen atom as an infinitely many-level atom including the continuum free states, which is known as the Kramers-Heisenberg formula. The discrepancy between the two formulae will be significant in the far off-resonance regions where the contribution from the $np(n > 2)$ states including the continuum states becomes considerable. Therefore, in order to obtain an accurate Gunn-Peterson profile it is essential to investigate the exact scattering optical depth of a medium with a high neutral hydrogen column density.

In this Letter, we present a faithful atomic physics that governs the scattering around Lyα by introducing the Kramers-Heisenberg formula and a simple fitting formula around Lyα. We compute the Gunn-Peterson trough profiles adopting a representative set of cosmological parameters with our choice of the reionization epoch and make

1

quantitative comparisons with previous works.

2. THE KRAMERS-HEISENBERG FORMULA

The interaction of photons and electrons is described by the second order time-dependent perturbation theory, of which the result is summarized as the famous Kramers-Heisenberg formula. As is well illustrated in a typical quantum mechanics text, it may be written as

$$
\frac{d\sigma}{d\Omega}(\omega) = \frac{r_0^2}{m_e^2\hbar^2} \left| \sum_I \left[\frac{\omega(\vec{p}\cdot\hat{\epsilon}^{(\alpha')})_{AI}(\vec{p}\cdot\hat{\epsilon}^{(\alpha)})_{IA}}{\omega_{IA}(\omega_{IA}-\omega-i\Gamma_I/2)} \right. \right.
$$
$$
\left. \left. - \frac{\omega(\vec{p}\cdot\hat{\epsilon}^{(\alpha)})_{AI}(\vec{p}\cdot\hat{\epsilon}^{(\alpha')})_{IA}}{\omega_{IA}(\omega_{IA}+\omega)} \right] \right|^2 \qquad (1)
$$

where $\hat{\epsilon}^{\alpha}, \hat{\epsilon}^{\alpha'}$ are the polarization vectors associated with the incident photon and outgoing photon, respectively, Γ_I is the radiation damping term associated with the intermediate state I, ω is the incident angular frequency, ω_{IA} is the angular frequency of the transition between I and the ground state A, and $r_o = e^2/(m_e c^2) = 2.82 \times 10^{-13}$ cm is the classical electron radius (e.g. Sakurai 1967).

Here, the electron is in the ground state A before scattering and de-excites to the same state. The summation (and integration) should be carried over all the intermediate states I including the infinite number of bound states and the free or continuum states. For hydrogen, the dipole moment matrix elements have been explicitly given using the recurrence relations of the hypergeometric function in many texts and in the literature (e.g. Berestetski, Lifshitz & Pitaevskii 1971, Bethe & Salpeter 1957, Karzas & Latter 1961).

In the blue part of Lyα, it is possible that the scattering atom may de-excite to the excited 2s state by re-emitting a photon with much lower frequency than the incident photon. This inelastic scattering or the Raman scattering is negligible near Lyα due to small phase space available for an outgoing photon. However, this process becomes important as the incident photon energy increases. In the range where the current work is concerned, the Raman scattering process is safely neglected.

Despite the existence of the explicit analytic expressions of each matrix element that constitutes the Kramers-Heisenberg formula for hydrogen, it is still cumbersome to use the formula as it is. Therefore, a simple fitting formula around Lyα will be useful for practical applications. Near resonance (1170 Å $< \lambda <$ 1410 Å), the Lorentzian function gives quite a good approximation

$$
\sigma(\omega) = \frac{3\lambda_\alpha^2}{8\pi} \frac{\Gamma_{2p}^2}{(\omega-\omega_\alpha)^2 + \Gamma_{2p}^2/4}, \qquad (2)
$$

where $\Gamma_{2p} = 6.25 \times 10^8$ s^{-1} is the radiation damping constant associated with the Lyα transition. In the long wavelength region ($\lambda > 1410$ Å), Gavrila (1967) provided the fitting polynomial for the Rayleigh scattering cross section, which is

$$
\sigma(\omega)/\sigma_T = 0.400(\omega/\omega_\alpha)^4 + 0.900(\omega/\omega_\alpha)^6
$$
$$
+ 12.6(\omega/\omega_\alpha)^{14}. \qquad (3)
$$

In particular, Ferland (2001) applied Gavrila's fit to his photoionization code 'Cloudy'.

In the case of the short wavelength region (1070 Å $< \lambda <$ 1170 Å), we provide a similar polynomial fit to the Kramers-Heisenberg formula

$$
\sigma(\omega)/\sigma_T = 1.62 \times 10^6 (\omega_\alpha/\omega)^4 + 5.88 \times 10^6 (\omega_\alpha/\omega)^3
$$
$$
+ 7.99 \times 10^6 (\omega_\alpha/\omega)^2 - 4.83 \times 10^6 (\omega_\alpha/\omega)
$$
$$
+ 1.09 \times 10^6. \qquad (4)
$$

The deviation of the fit is within 5 per cent from the true Kramers-Heisenberg formula.

In Fig. 1 we show the scattering cross section from the Kramers-Heisenberg formula by the solid line and by the dotted line we represent the fit. The behavior near resonance is depicted in the bottom panel, because the cross section changes very steeply. It is apparent that the scattering cross section is excellently approximated by the Lorentzian. However, in the wavelength range considered in this Letter, the radiation damping is completely negligible, and the curve shown in the figure is simply proportional to $\Delta\omega^{-2} = (\omega - \omega_{Ly\alpha})^{-2}$. The deviation is slightly anti-symmetric with respect to the line center in the sense that the cross section in the blue part is smaller than the Lorentzian and in the red part it is larger than the Lorentzian.

Therefore, 1 per cent of deviation of the Lorentzian from the Kramers-Heisenberg formula is seen at a wavelength shift of $\Delta\lambda = \lambda - \lambda_\alpha = \pm 3.3$ Å, for which the corresponding cross section $\sigma = 3.8 \times 10^{-21}$ cm^2. This indicates the accuracy of the Voigt profile fitting applied to quasar absorption systems, where the accuracy is more than 99 per cent when the absorbing medium is characterized with the H I column density smaller than 3×10^{20} cm^{-2}.

Further away from the line center, the cross section in the blue part decreases very steeply till $\lambda \sim 1100$ Å, but the decrease of the cross section in the red part is rather gradual and eventually becomes proportional to ω^4, which corresponds to the classical result.

Fig. 1 also shows the comparison of the Kramers-Heisenberg formula and the heuristic formula

$$
\sigma_P(\omega) = \frac{3\lambda_\alpha^2}{8\pi} \frac{\Gamma_{2p}^2(\omega/\omega_\alpha)^4}{(\omega-\omega_\alpha)^2 + \Gamma_{2p}^2(\omega/\omega_\alpha)^6/4} \qquad (5)
$$

introduced by Peebles (1993).

The ω^4 dependence in the limit $\omega \ll \omega_\alpha$ is obtained as a result of the closure relation, which is apparent in the both formulae. However, the Kramers-Heisenberg formula gives about twice larger scattering cross section than σ_P does. This deviation is easily noted when the oscillator strength of the Lyα transition is $f_{Ly\alpha} = 0.42$. The scattering cross section in the far red region is contributed from all the p states and the oscillator strength is a good measure of the contributions of each individual excited state. This implies that the 2p state contribution is comparable to the total contributions from the remaining states in the low energy limit.

3. GUNN-PETERSON TROUGH PROFILES WITH THE KRAMERS-HEISENBERG FORMULA

We compute the Gunn-Peterson optical depth defined by

$$
\tau_{GP} = \int_{z_{rei}}^{z_s} dz \, \frac{dl}{dz} \sigma[\nu = c(1+z)/\lambda_{obs}] \, n(z), \qquad (6)
$$

with the Kramers-Heisenberg formula and make comparisons with previous works performed by Madau & Rees (2000) (see also Miralda-Escudé 1998). Here, λ_{obs} is the observed wavelength, z_{rei}, z_s are the redshifts of the complete reionization of the universe and the reionizing source, and $n(z) = n_0(1+z)^3$ is the homogeneous neutral hydrogen density at redshift z. We choose $z_{rei} = 6$, $z_s = 7$ as in Madau & Rees (2000), but do not consider the proximity effect of the ionizing source. The Gunn-Peterson optical depth can be written as

$$\tau_{GP} = N_{0\,HI} \int_{z_{rei}}^{z_s} dz \; \sigma[\nu = c(1+z)/\lambda_{obs}]$$
$$\times (1+z)^2/[\Omega_M(1+z)^3 + \Omega_\Lambda]^{1/2}, \qquad (7)$$

where Ω_M, Ω_Λ are the density parameters due to matter and the cosmological constant and the characteristic hydrogen column density

$$N_{0\,HI} \equiv n_0 \; c \; H_0^{-1}. \qquad (8)$$

We choose the present Hubble constant and the hydrogen number density $H_0 = 50$ km s^{-1} Mpc^{-1}, $n_0 = 2.4 \times 10^{-7}$ cm^{-3} so that $N_{0\,HI} = 4.3 \times 10^{21}$ cm^{-2}.

In Fig. 2, we show the Gunn-Peterson transmission coefficient $T_{GP} \equiv e^{-\tau_{GP}}$. We plot T_{GP} for the case $\Omega_M = 1, \Omega_\Lambda = 0$ in the top panel and the same quantity for an accelerated expanding universe $\Omega_M = 0.35, \Omega_\Lambda = 0.65$ in the bottom panel. In terms of the characteristic Gunn-Peterson optical depth $\tau_{0\,GP}$ defined as

$$\tau_{0\,GP}(z_s) \equiv \frac{3\lambda_\alpha^3 \Gamma_{2p} n(z_s)}{8\pi H(z_s)}, \qquad (9)$$

our choice of parameters in the case of the top panel yields the value of $\tau_{0\,GP} = 3 \times 10^5$ at $z_s = 7$ as was adopted in the work of Madau & Rees (2000).

The horizontal axis represents the logarithm of the normalized wavelength ratio δ defined as

$$\delta \equiv \frac{\lambda_{obs}}{\lambda_\alpha(1+z_s)} - 1, \qquad (10)$$

from which $\delta = 0$ corresponds to the resonance wavelength of Lyα. By the dotted lines we present the Gunn-Peterson transmission coefficient obtained using the scattering cross section given by Eq. (5). The deviation between the two formulae is notable around $\delta = 10^{-2}$, where the deviation is about 3 per cent in the top panel and 5 per cent in the bottom panel. The Peebles approximation turns out to be pretty good for contemporary application.

The deviation between the two formulae will increase as n_0 or $N_{0\,HI}$ increases, because the discrepancy of the Kramers-Heisenberg formula and Eq. (5) becomes larger as the frequency is further away from the line center. Near resonance, both formulae are excellently approximated by the same Lorentzian. Therefore, no significant deviation is expected when the neutral medium is of low column density $\lesssim 10^{21}$ cm^{-2}. It is notable that an accurate treatment of atomic physics is more important in an accelerated expanding universe where the univere was more compact than the universe without the cosmological constant.

4. SUMMARY AND DISCUSSION

In this Letter, we have investigated the behavior of the scattering cross section around Lyα in a quantitative way, where the deviation from the Lorentzian becomes significant as the incident frequency gets further away from the line center. Therefore, in an analysis of the Gunn-Peterson trough profile, which is associated with a neutral medium with a high H I column density, an inaccurate treatment of the atomic physics of hydrogen may introduce significant errors in estimating important cosmological parameters including the epochs of the emergence of the first objects and the completion of the reionization of the universe.

Voigt profile fitting has been very successfully applied to quasar absorption systems with a broad range of H I column densities. However, the deviation of the true scattering cross section from the Lorentzian exceeds 1 per cent when the relevant column density becomes $N_{HI} \geq 3 \times 10^{20}$ cm^{-2} that is the typical column density of a damped Lyα absorber. This is especially important in some damped Lyα systems that may possess $N_{HI} > 10^{21}$ cm^{-2} (e.g. Turnshek & Rao 1998). However, it should be noted that the damping constant Γ_{2p} is so small compared with the scale relevant in this work, the cross section is effectively of the form $\propto \Delta\omega^{-2} = (\omega - \omega_\alpha)^{-2}$. Therefore, the absorption profile is irrelevant to the exact value of the radiation damping term, which means that the term 'damped Lyα absorption' is a misnomer.

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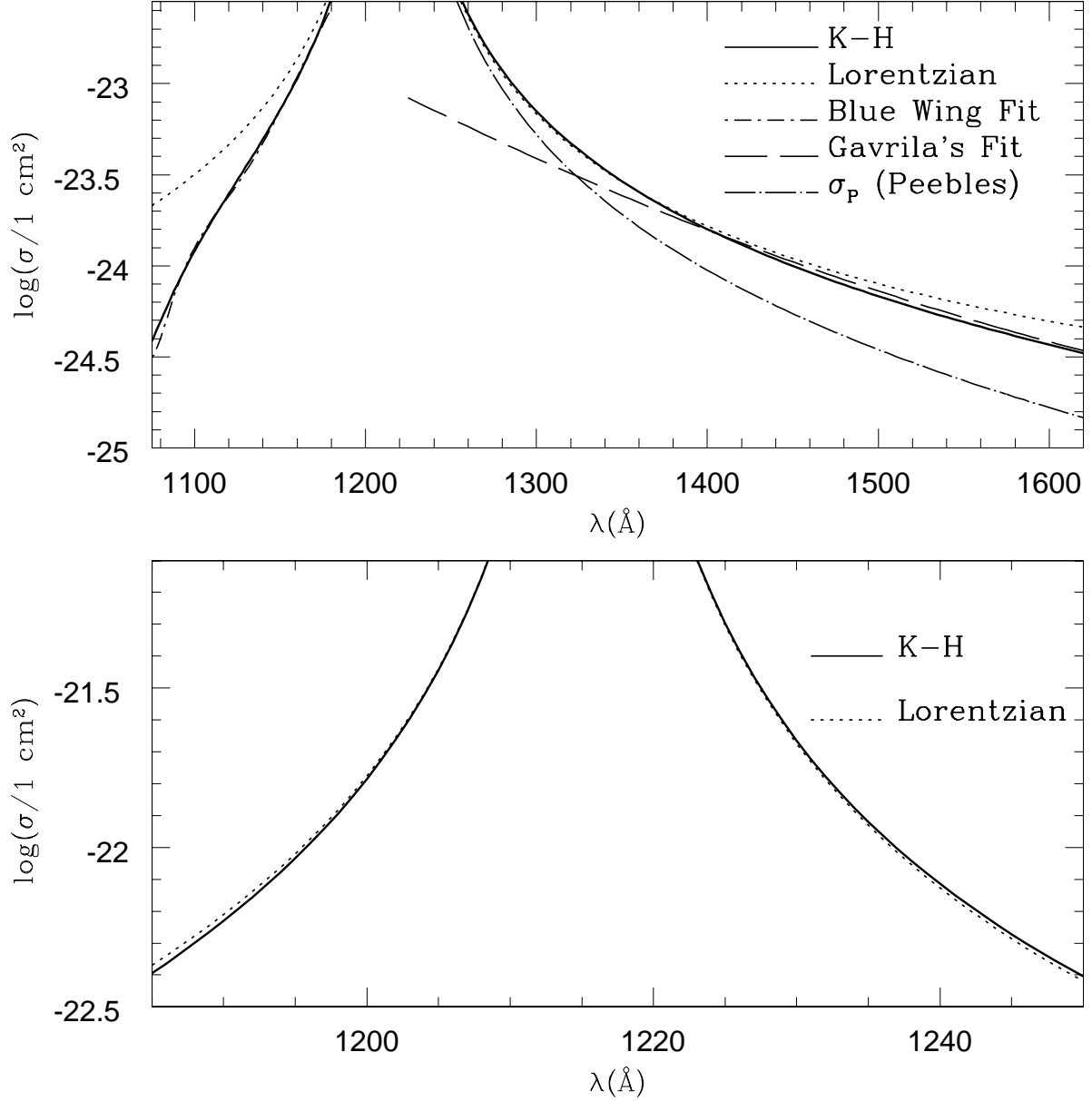Turnshek, D. A., & Rao, S., 1998, ApJ, 500, L115

FIG. 1.— The scattering cross section around Lyα. The solid line represents the accurate, fully quantum mechanical cross section known as the Kramers-Heisenberg formula. The dotted line represents the Lorentzian given by Eq. (2), which gives an excellent approximation near the line center. The long dashed line represents the fitting formula provided by Gavrila (1967), of which the approximation is valid for $\lambda > 1400$ Å. The dot-dash line represents our fit to the Kramers-Heisenberg formula in the blue part given in Eq. (4). The dot-long dash line represents the cross section obtained from Eq. (5), which is inaccurate by a factor of two in the far red wing region and accurate near the line center. In the bottom panel, we plot the cross section obtained from the Kramers-Heisenberg formula (solid line) and the Lorentzian Eq. (2). The cross section is asymmetric relative to the line center in the sense that the cross section in the blue part is smaller than in the red part.
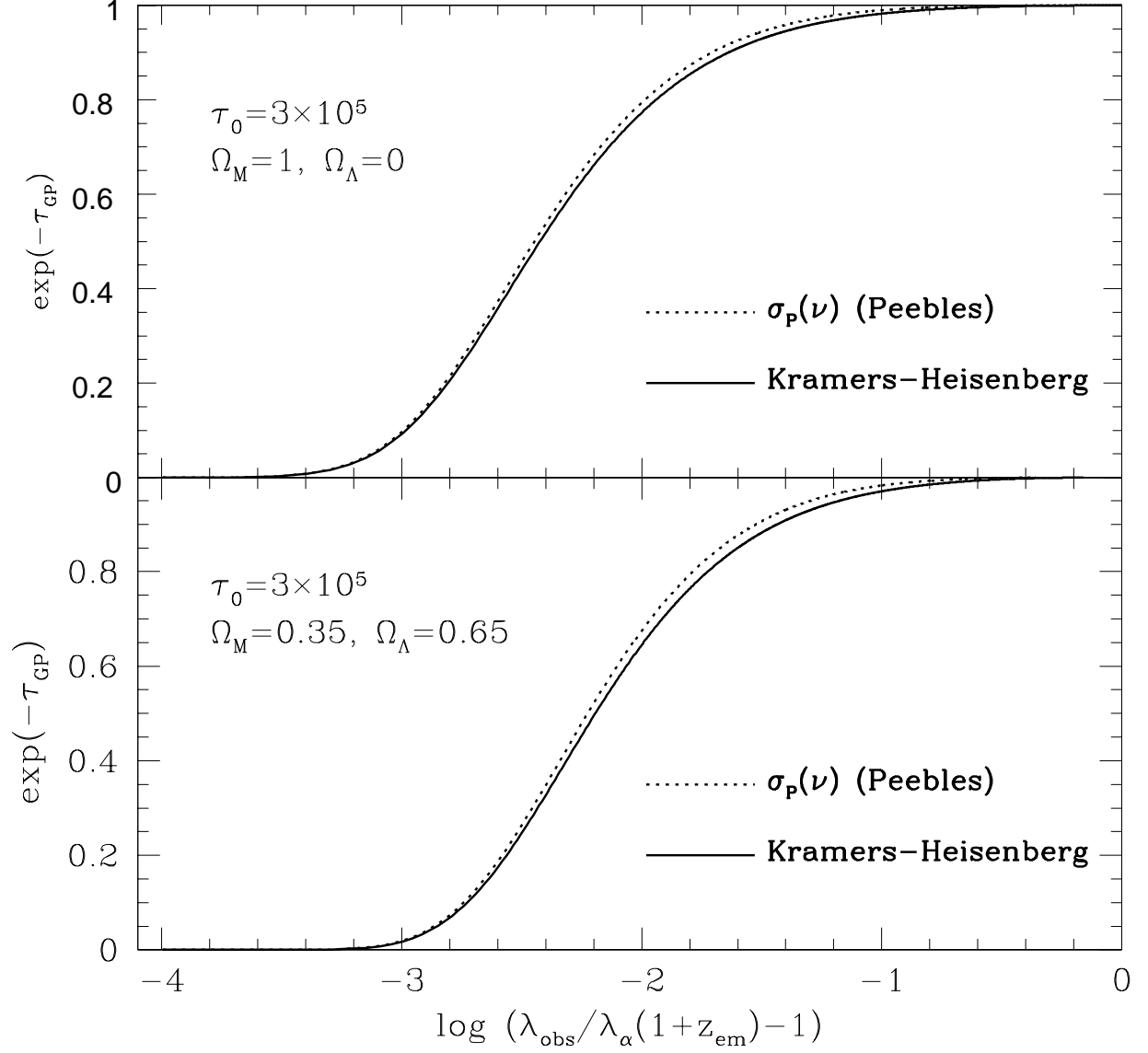
FIG. 2.— The Gunn-Peterson transmission coefficient $T_{GP} \equiv e^{-\tau_{GP}}$ for $\Omega_M = 1, \Omega_\Lambda = 0$ (top panel) and for $\Omega_M = 0.35, \Omega_\Lambda = 0.65$ (bottom panel). The solid lines represent the values obtained using the Kramers-Heisenberg formual and the dotted lines are for the values from the cross section σ_P introduced by Peebles (1993). The present Hubble constant and the hydrogen number density are chosen to be $H_0 = 50$ km s^{-1} Mpc^{-1}, $n_0 = 2.4 \times 10^{-7}$ cm^{-3} so that $N_{0\,HI} = n_0 c H_0^{-1} = 4.3 \times 10^{21}$ cm^{-2}.